Friction and Lubrication at the Nanoscale

The DOE **C**enter of Excellence for the
Synthesis and **P**rocessing of Advanced Materials

Center Review

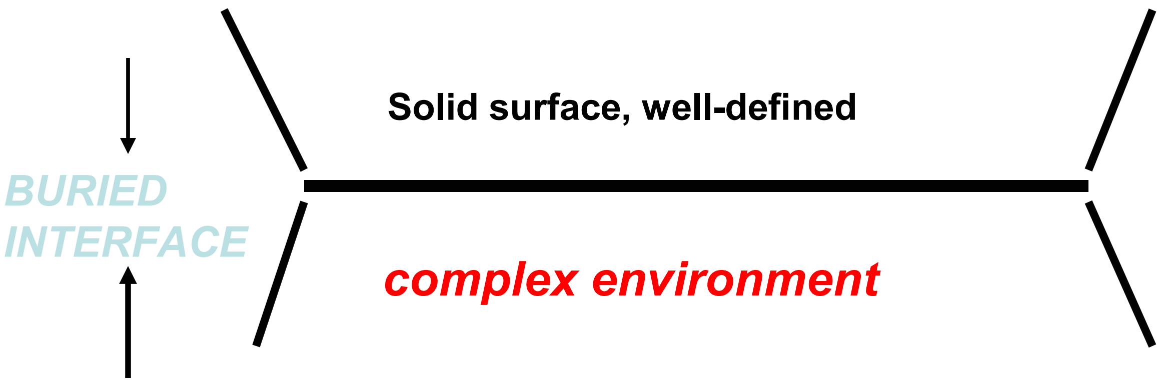
DOE, Germantown, MD. Friday June 4, 2004

Yehuda Braiman

Oak Ridge National Laboratory

ARGONNE NATIONAL LABORATORY
Los Alamos NATIONAL LABORATORY
Pacific Northwest National Laboratory
BERKELEY LAB
University of Illinois
Frederick Seitz Materials Research Laboratory
OAK RIDGE NATIONAL LA
Sandia National Laboratories

THE TRIBOLOGY PROBLEM



Driven by shear field, chemical reactions, and complexity in the surface potential

Energy and technology relevance: lubrication; transportation; defense programs; MEMS; biosensors; microfluidics; chemical reactivity at and near surfaces; flow processing of ceramics and polymers; formation and adhesive characteristics of coatings; fundamentals of solid-fluid interface science; the science and technology of interacting surfaces in relative motion.

Main tasks of the group

TASK 1. Synthesis & processing of new surface coatings

FS-MRL, ANL, LANL, SNL/NM

TASK 2. New theoretical and computational advances

SNL/NM, PNNL, ORNL

Unifying systems

TASK 3. New spectroscopic and nanoprobe methods

FS-MRL, LANL, SNL/NM, LBNL, UCSD

TASK 4. New insights into relations between nanoscale, microscale, and macroscopic tribology

FS-MRL, ORNL, ANL, UCSD

Experimental and Computational Lubrication at the Nanoscale
Report of the First Annual Meeting
Held at SNL/NM on March 14, 2003

This first meeting of the entire group since the S & P Center was awarded also attracted extensive outside participation. In attendance were:

ANL:	Ali Erdemir, Orlando Auciello
LANL:	Jeanne Robinson
PNNL:	James Cowin
SNL/NM:	Gary Grest, Jack Houston, Marten de Boer, Mike Kent,Mike Chandross, Mark Stevens, Tom Friedmann, Mike Dugger, George Samara
ORNL:	Yehuda Braiman, Peter Cummings, Peter Blau
LBNL:	Miquel Salmeron
UCSD:	Sunhil Sinha
UI/FS-MRL:	Steve Granick

Proposed Areas of Focus:

1. ***Confined water and lubrication: SAM coatings, water penetration, chemical degradation***

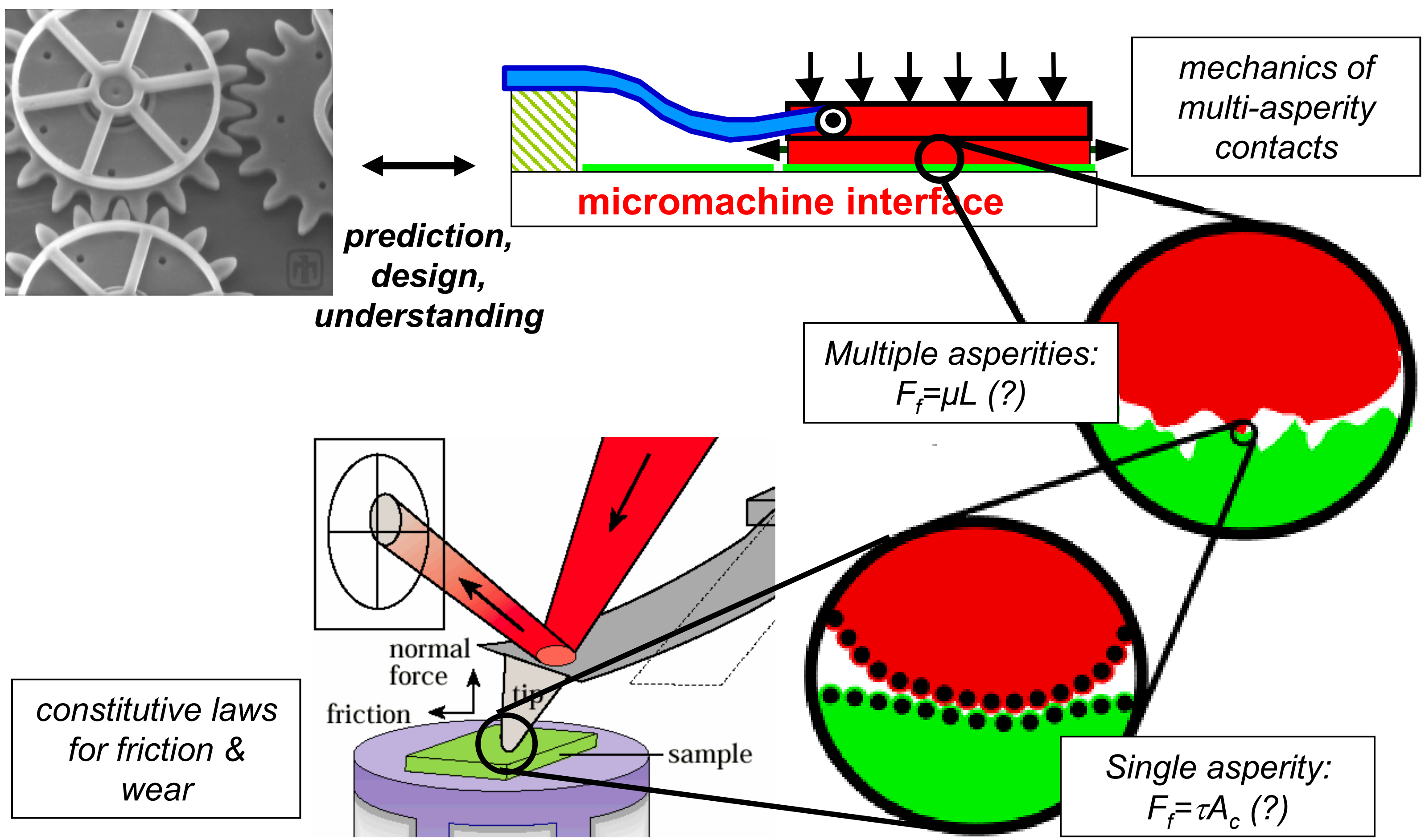
2. ***Confined non-polar fluids and lubrication***

3. ***Patterned surfaces, controlled chemical and topographical heterogeneity***

New insights into relations between nanoscale, microscale, and macroscopic tribology

ANL, FS-MRL, ORNL, UCSD, SNL, U Wisconsin

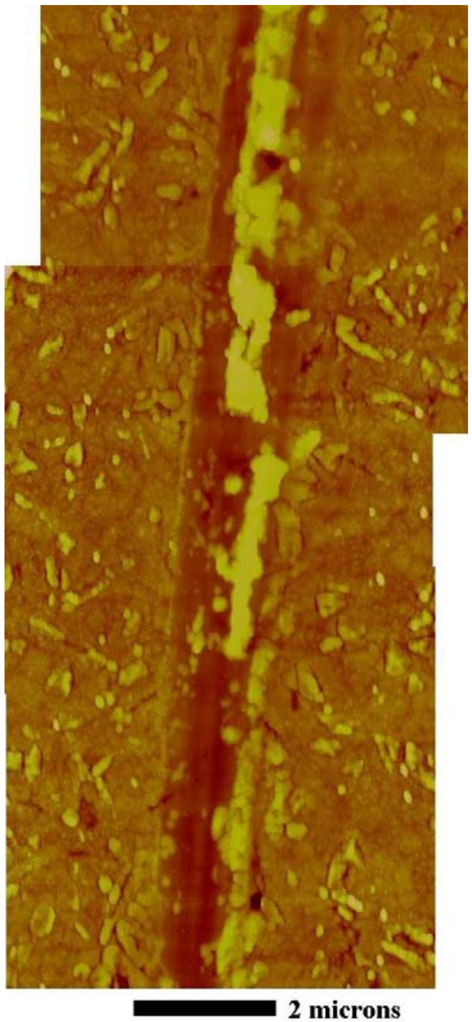
A multi-scale understanding of friction is developed through experiment and modeling



M. DeBoer (SNL), R. Carpick (U. Wisconsin)

High resolution AFM images of the worn MEMS countersurface

Significant variations in surface topography along wear track



75 nm height scale

Measure topography of MEMS surfaces with high resolution using AFM

Measure frictional constitutive behavior of MEMS surfaces using AFM (silicon, nanocrystalline diamond)

Combine this information with multi-asperity contact models to predict friction, wear, and reliability in MEMS

compare to an actual MEMS friction test device

never done before for MEMS surfaces!

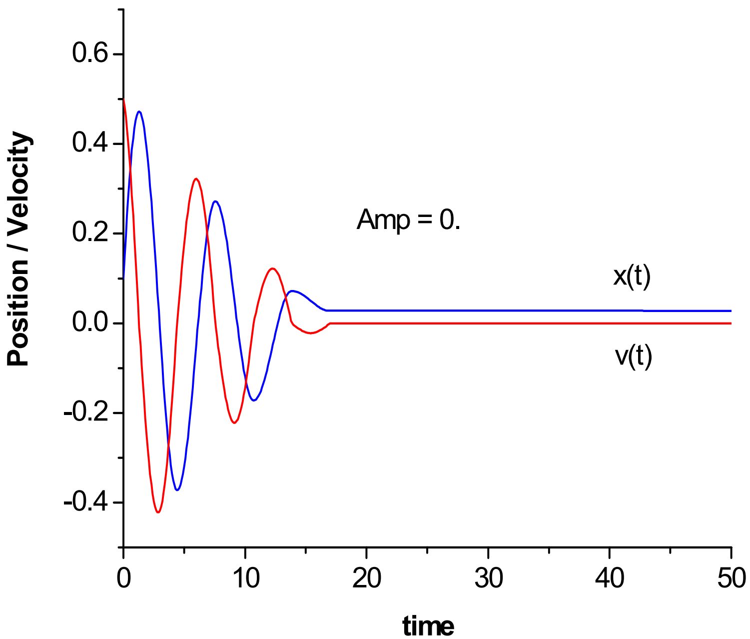
Determine how best to tailor MEMS surfaces to reduce friction & wear

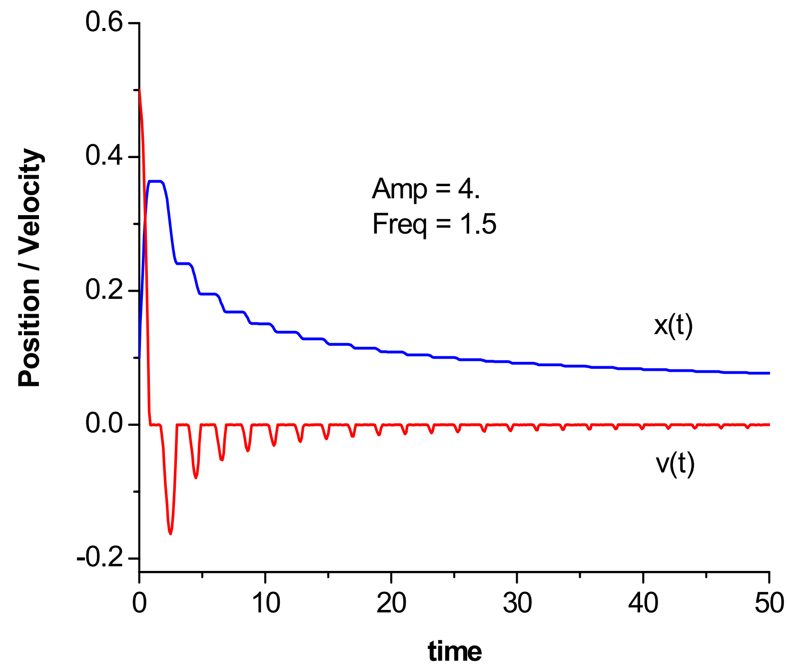
M. De Boer (SNL), R. Carpick (U. Wisconsin)

Control of Friction of the Inchworm

$$m\ddot{x}+b\dot{x}+\mu\left(mg+\alpha V^{2}(t)+\frac{A}{12\pi d_{0}^{3}}\times Area-k_{0}g_{0}\right)\times\mathrm{sgn}(\dot{x})+kx=0$$

Oscillatory control: $V(t)=A\sin(\omega_e t)$





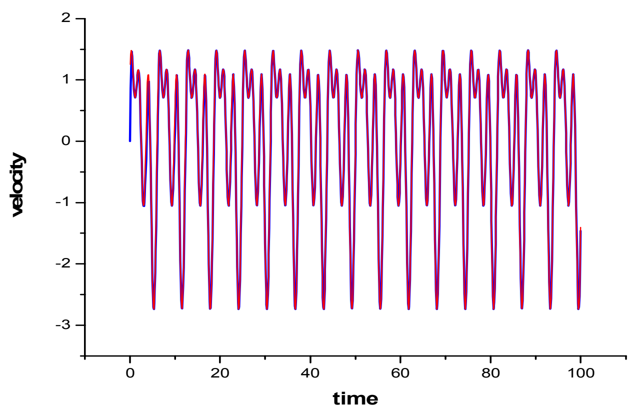
NonLipschitzian Friction Control of the Inchworm

Equation of motion in dimensionless units in the presence of control:

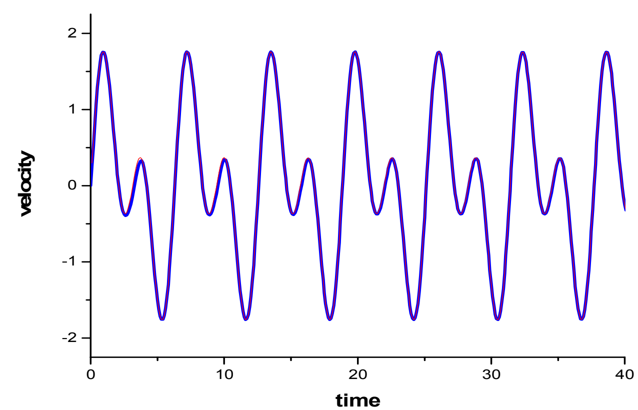
$$\frac{d^2x}{d\tau^2} + 0.026\frac{dx}{d\tau} + 0.0071\mu \times \mathrm{sgn}\left(\frac{dx}{d\tau}\right) + 0.3(0.0363x^3 + 0.254x^2 + 3.039x) = C(t) \quad (8)$$

$$C(t) = \alpha\left(F(t)_{target} - \frac{dx}{dt}\right)^{1/\beta}$$

$$F(t)_{target} = A[\sin(\omega t) + \sin(2\omega t) + \cos(3\omega t)]$$



$$F(t)_{target} = A\sin(\omega t) + A\sin(2\omega t)$$



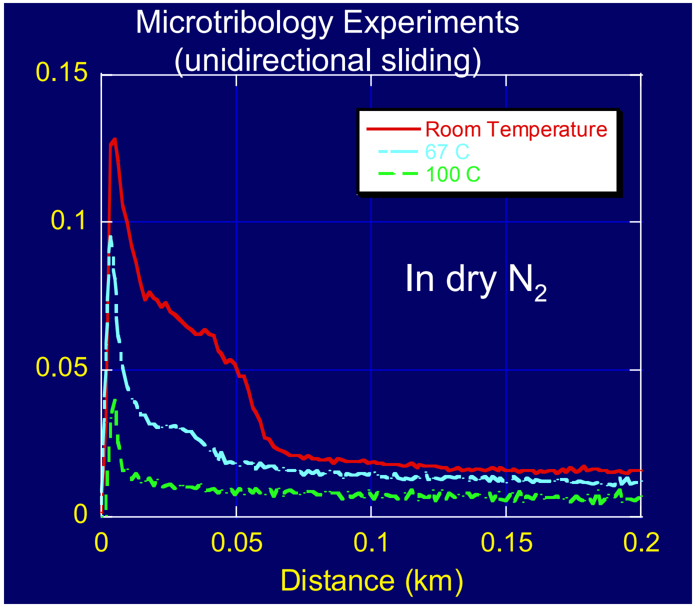
Synthesis & processing of new surface coatings

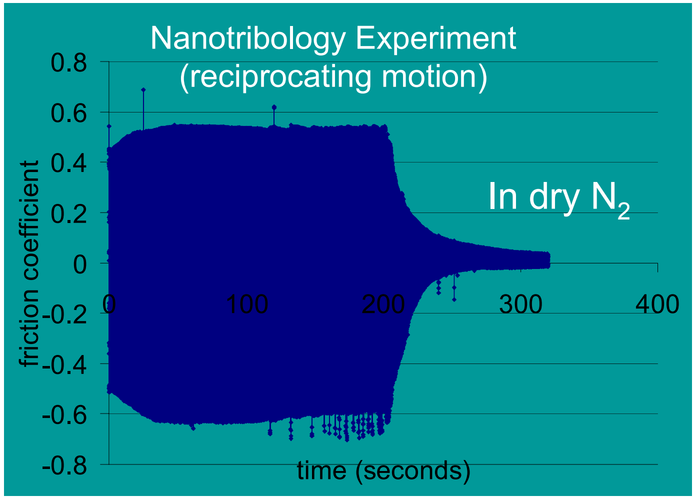
FS-MRL, ANL, LANL, SNL/NM, UCSD

Ultralow Friction

ANL, ORNL, SNL, U. Wisconsin

EFFECTS OF SURFACE ADSORBATES ON FRICTION AND WEAR OF CARBON FILMS



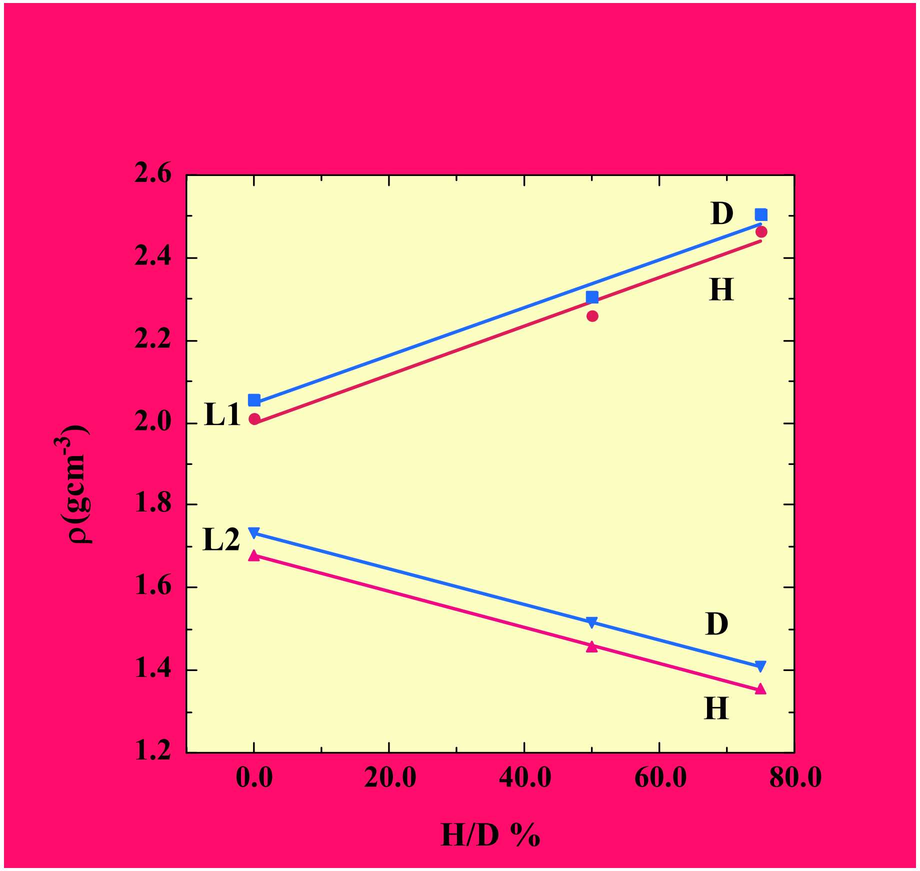


Recent systematic work at Argonne National Laboratory has led to the development of a series of diamondlike carbon films that can provide friction coefficients of 0.003 to 0.006 when tested in both the micro- and nano-scale tribotest machines as shown in these Figures. However, the initial or break-in friction is rather high and believed to be caused by surface adsorbates. To understand the true mechanism of high initial friction, we attempted to analyze the chemical and physical nature of such adsorbates using both the neutron and x-ray reflectivity methods.

A. Erdemir and J. Johnson/ANL
Sunil K. Sinha/UCSD

ARGONNE NATIONAL LABORATORY

Neutron reflectivity (NR) Results



NR revealed a higher density (2 - 2.5 g.cm-3) top surface layer that is ~ 3 nm thick. The presence of such layers on sliding DLC surfaces may in part be responsible for high initial friction. As these layers are mechanically removed or worn out during repeated sliding passes, the friction becomes very low (e.g., 0.005) at steady states.

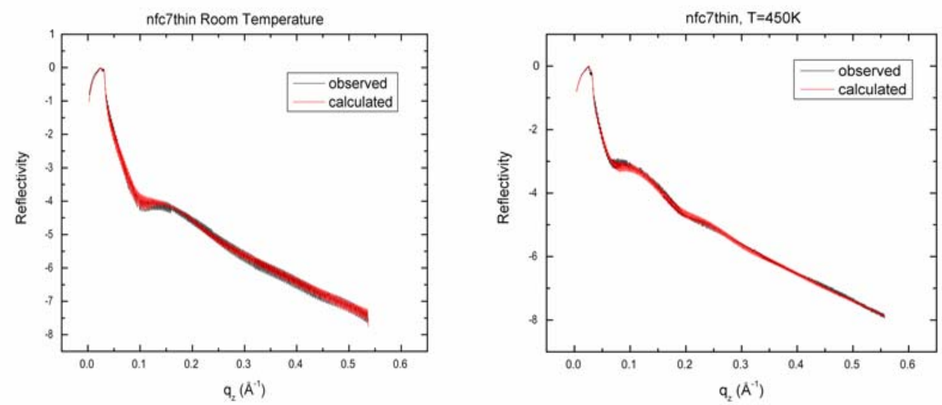
The NR measurements were performed on deuterated and hydrogenated films as a function of neutron momentum perpendicular to the carbon surface in air at room temperature. The scans were taken at angles of 0.5, 1.0, and 1.5 degrees and the transmitted and reflected beams were detected with a two-dimensional position sensitive detector.

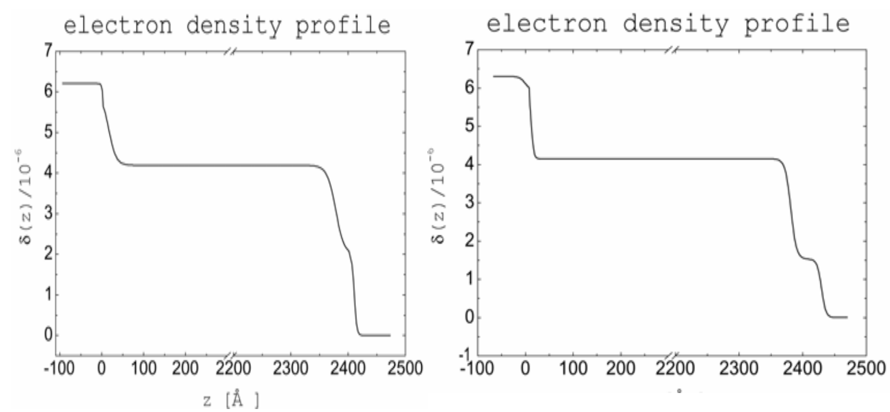
A. Erdemir and J. Johnson/ANL
Sunil K. Sinha/UCSD

X-Ray Reflectivity Measurements at Synchrotron

X-Ray Reflectivity Curves yield the Electron density Profiles of the films. Model density profiles are fitted to the reflectivity data.

Analysis of X-Ray reflectivity measurements from these films reveals internal (electron) density profiles of films, showing a 3 nm dense diamond-like layer (sp3 bonding) near the Si surface, a bulk film showing sp2 bonding, and a 1-3 nm less dense but smooth layer on the film surface, which becomes thicker when the sample is taken to higher temperatures.
(0 measures the position of the Silicon substrate surface)





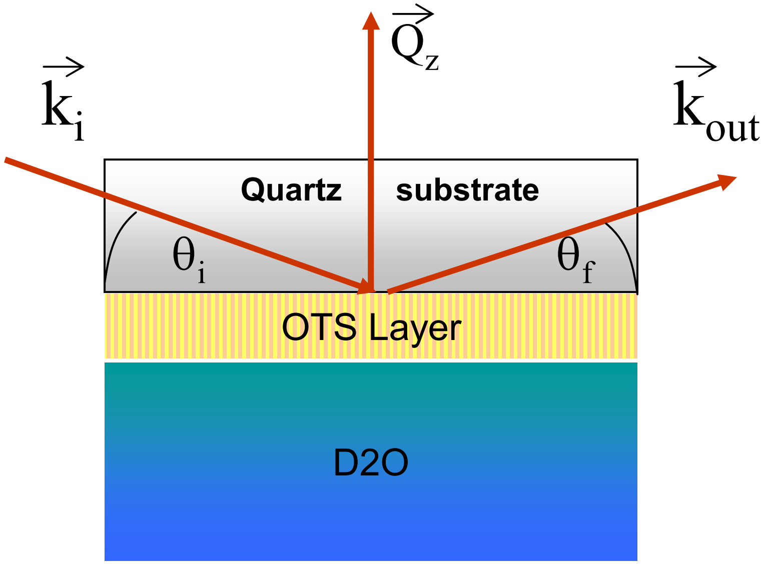
300K

450K

Neutron Reflectivity of OTS and Patterned OTS Films Swelled in D_2O

Neutron scattering is a powerful tool for surface studies.

- Film thickness
- Coverage
- Roughness



$$\theta_i = \theta_f$$

Advantages:

Better Contrast
Low absorption / variety of interfaces
Non-destructive
Length scale 10-5000Å

Disadvantage:

Model system

$$q_z = \Delta k = |\bar{k}_f - \bar{k}_i| = 4\pi \sin\theta/\lambda$$

E.B. Watkins et al., LANL

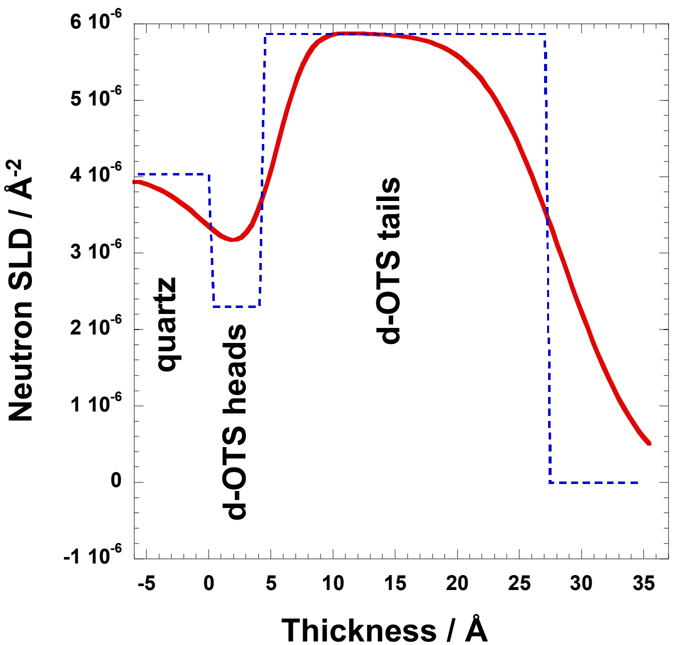
Los Alamos NATIONAL LABORATORY

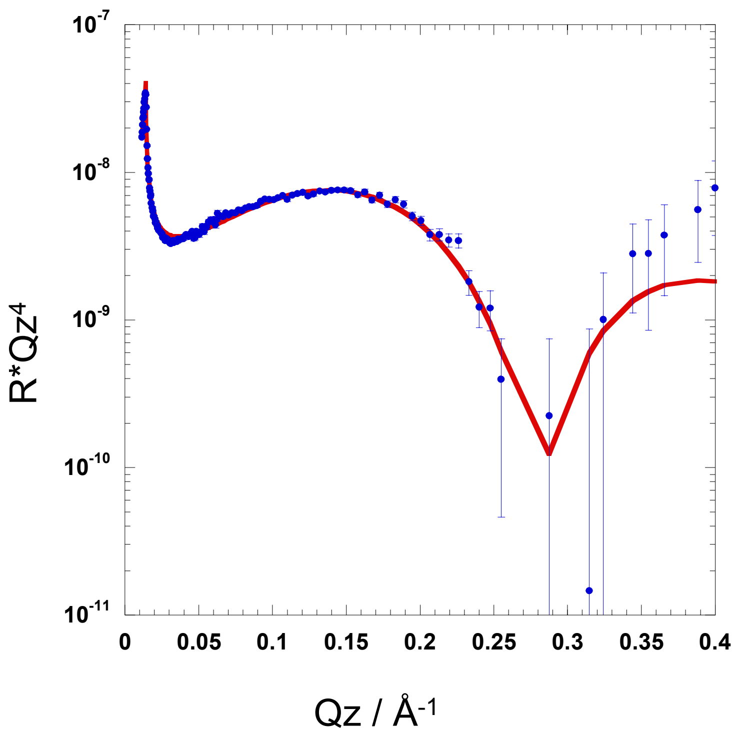
Neutron Reflectivity of d-OTS in air

By using deuterated OTS, good contrast can be achieved between the head and tail for a monolayer film in air.

•The silane head groups appear as a less dense region of silica

•d-OTS packing density of 1 molecule / 26 Å^2





Box Model Fit parameters for the d-OTS monolayer in air

	Thickness / Å	Neutron SLD / Å^{-2}	Roughness / Å rms
d-OTS tails	23	5.9e-6	5
d-OTS heads	4	2.3e-6	2
Quartz		4.0e-6	4

J. Robinson et al

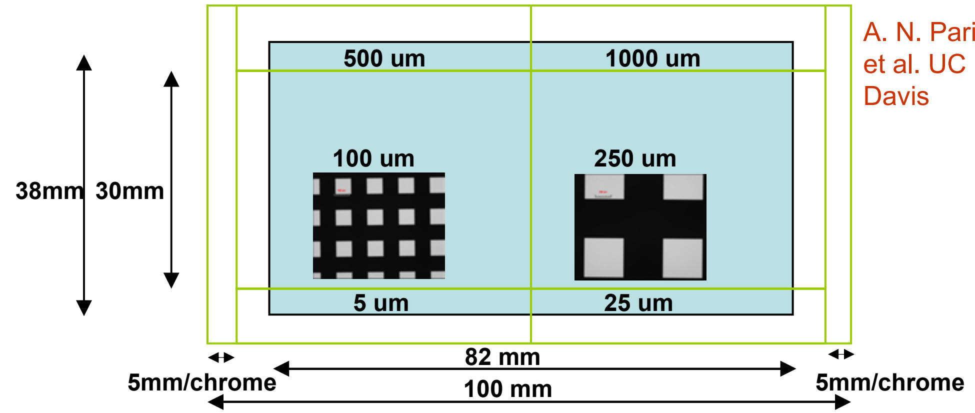
Los Alamos NATIONAL LABORATORY

Neutron Reflectivity of OTS and Patterned OTS in D_2O

The OTS samples were self-assembled on quartz substrates and measured against D_2O.

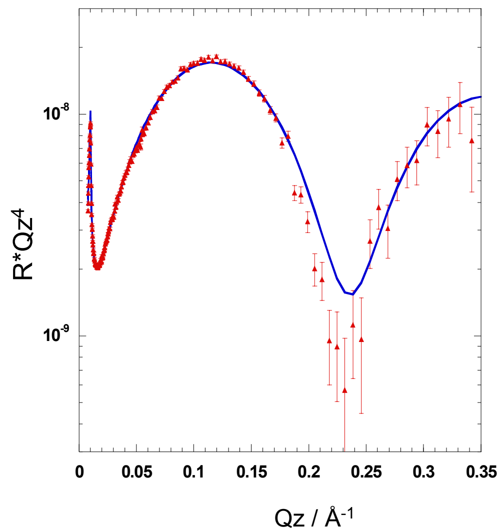
•OTS packing density of 1 molecule / 22 $Å^2$

•80% coverage of OTS in the patterned sample



A. N. Parikh, et al. UC Davis

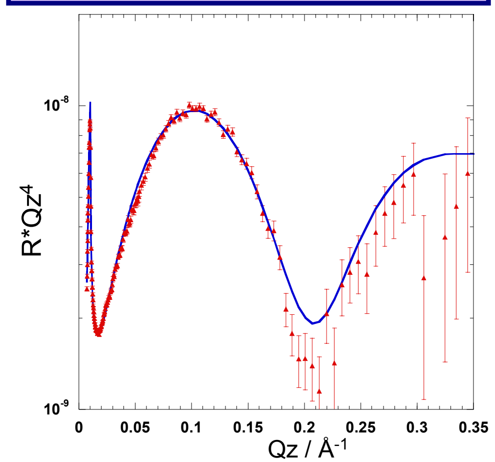
Neutron Reflectivity Data and Model Fit for an OTS monolayer



	Thickness / Å	Neutron SLD / $Å^{-2}$	Roughness / Å rms
Quartz		4.1e-6	3
OTS	26	-3e-7	2
D_2O		6.2e-6	

E. B.Watkins, J. Majewski, et al. LANL

Neutron Reflectivity Data and Model Fit for a patterned OTS monolayer



	Thickness / Å	Neutron SLD / $Å^{-2}$	Roughness / Å rms
Quartz		4.1e-6	5
OTS	29	1e-6	2
D_2O		6.2e-6	

Los Alamos
NATIONAL LABORATORY

New spectroscopic and nanoprobe methods

FS-MRL, ANL, LANL, SNL/NM

Optical Studies of Liquids in the Surface Forces Apparatus

***Granick*:** fluorescence, confocal Raman

***Salmeron*:** sum-frequency-generation

- Macro-scale (10^{10} molecules)
  - Force measurements
- **Meso-scale? (100s of molecules)**
- **Nano-scale?? (10s of molecules)**

Force Measurements (Classical tribology)

(+) Powerful and sensitive (10 pJ)
(+) Application of shear and normal force
(+) Characterization of numerous systems (liquids, polymers)
(-) Structure must be "inferred"
(-) Perturbation/relaxation technique involving huge ensemble averaging

Optical Measurements

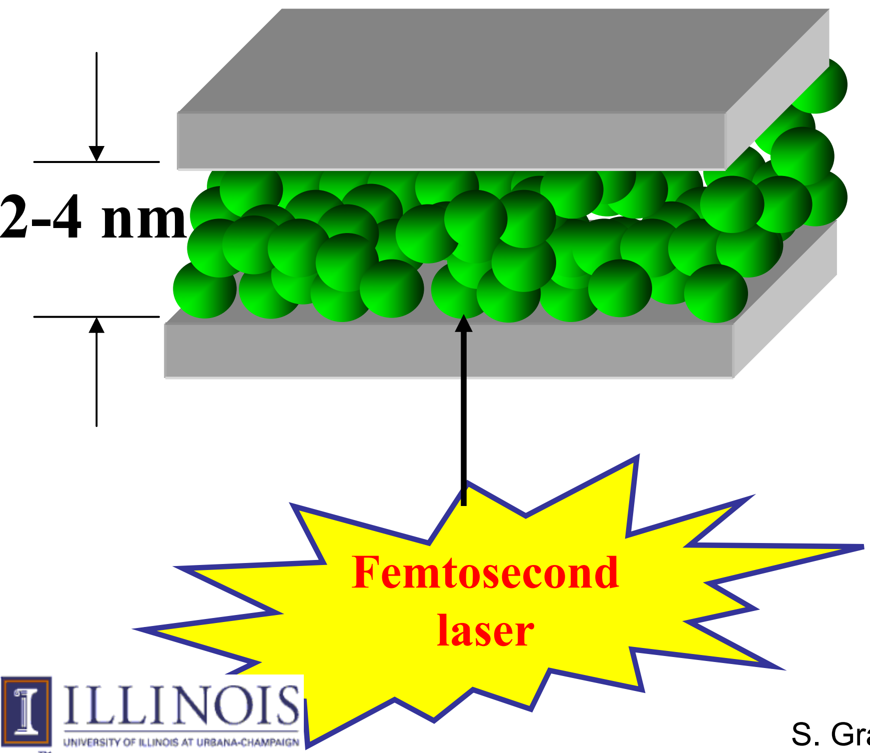
- Highly sensitive (single molecule response)
- Little perturbation of the system
- Capable of probing dynamics and heterogeneity

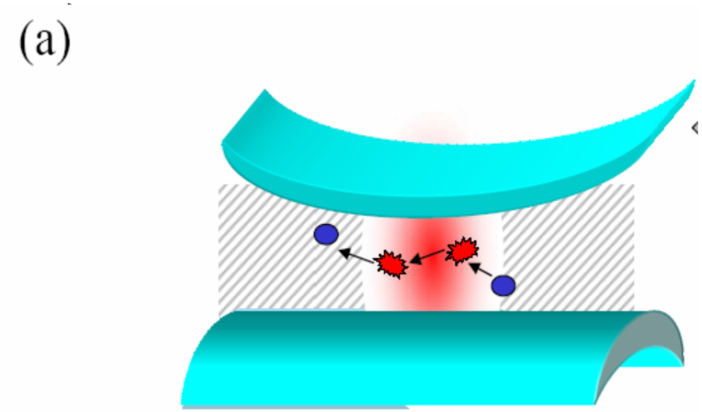
Local Viscosity and Environment on the Nanometer Scale

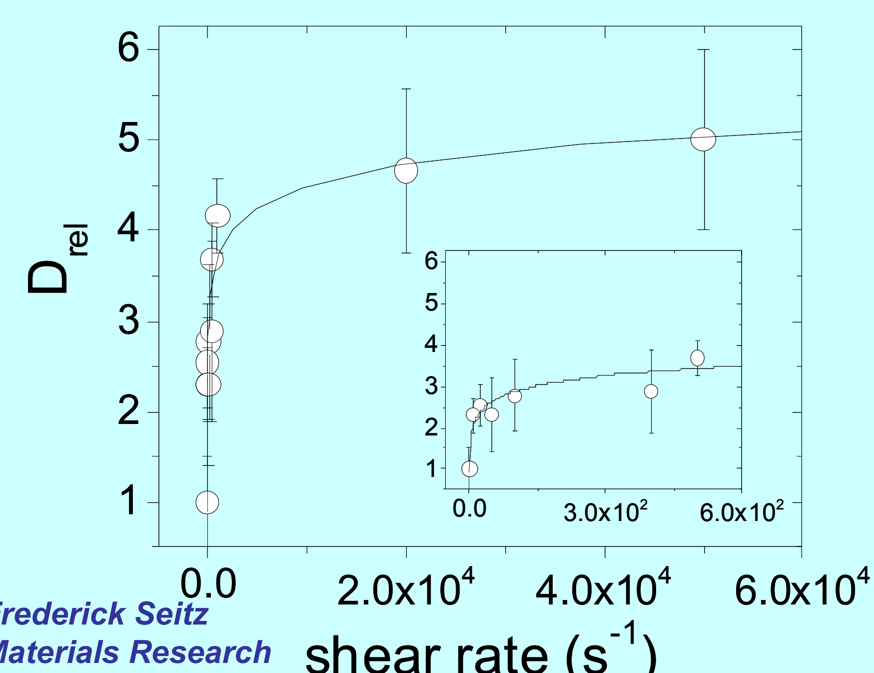
BURIED INTERFACE

complex environment (intentionally or not)

Surface, well-defined







Frederick Seitz Materials Research Laboratory

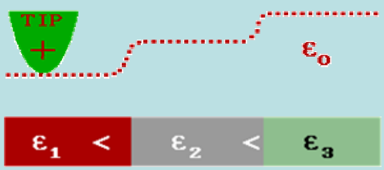
ILLINOIS
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

S. Granick

Combination of AFM techniques to study water interaction with organic monolayers

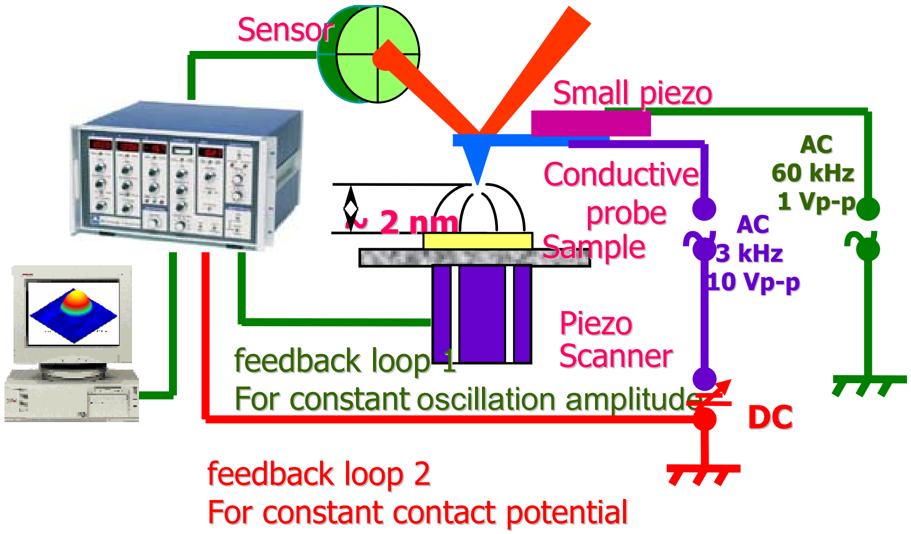
Electrostatic imaging
(Scanning Polarization Force Microscopy)

Contrast

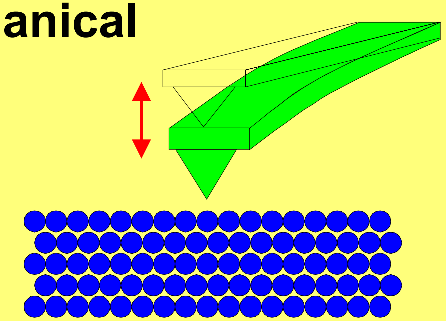


$$F_{pol} \approx \frac{\varepsilon_i - \varepsilon_o}{\varepsilon_i + \varepsilon_o}$$

Dielectric Spectroscopy
Freq. Dependence of $\varepsilon(\omega)$

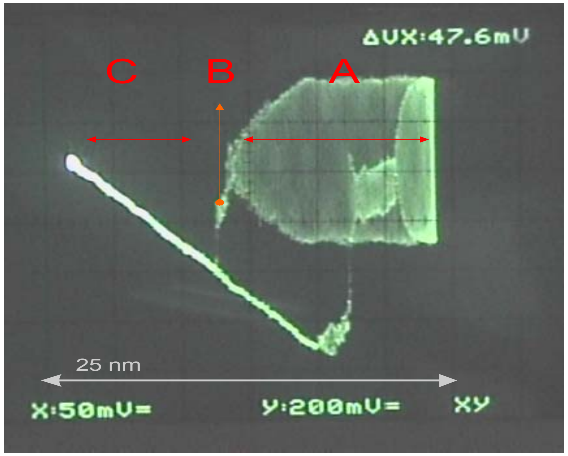


Mechanical



Non-contact AFM based on resonance oscillation of the lever.

Imaging at point between A and B, before contact



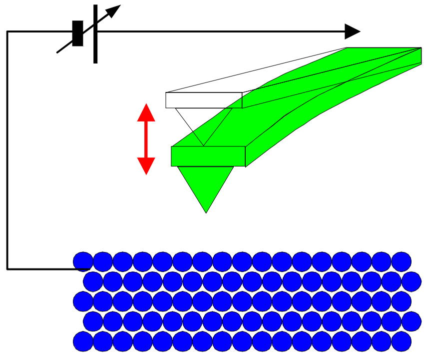
Miquel Salmeron. Lawrence Berkeley National Laboratory

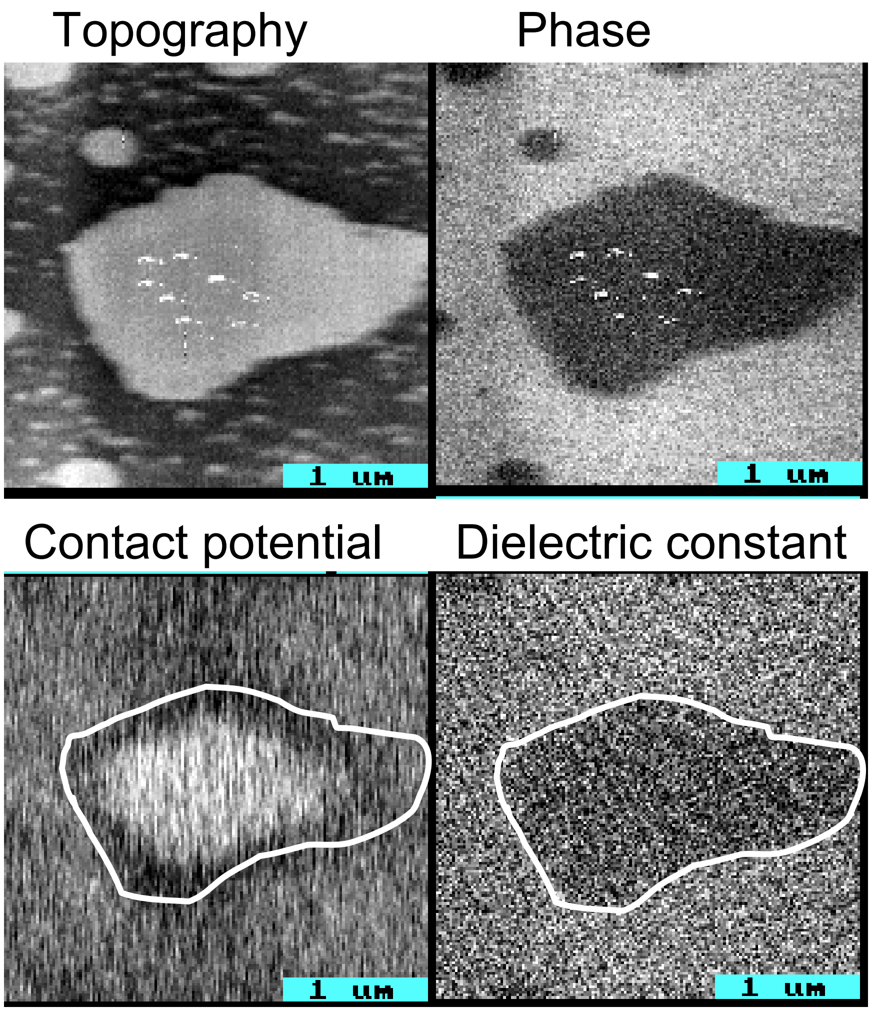
Result 1: **alkylsilane islands on mica**

Double feedback imaging: 1st mech. resonance amplitude

2nd contact potential

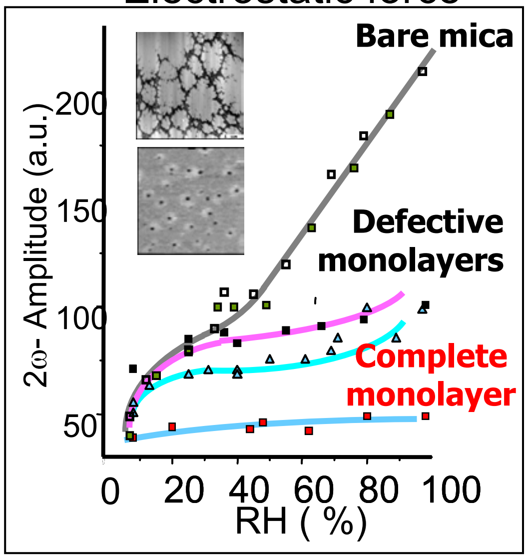
4 simultaneous images



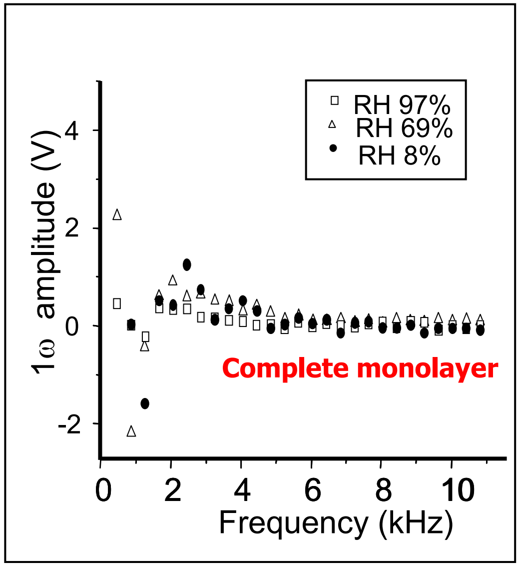


Result 2: SPFM of Silanes (C16, C18) on mica demonstrates that water does not penetrate to the interface except at defects and domain boundaries

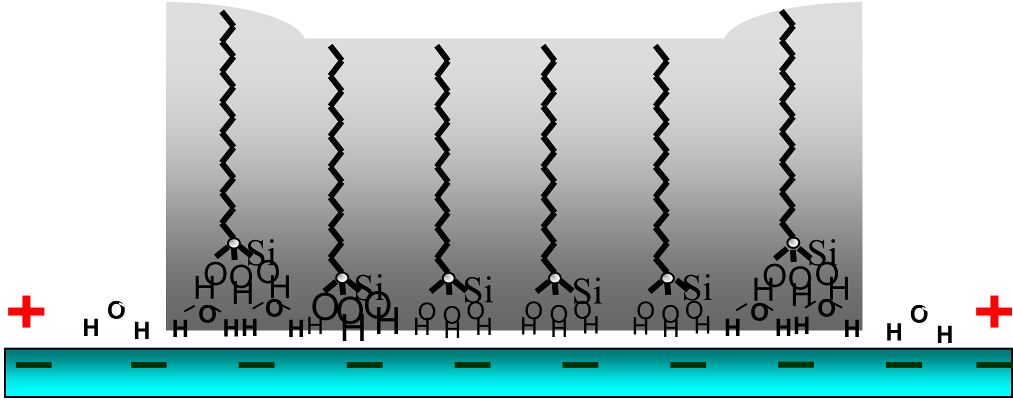
Electrostatic force



Contact potential difference

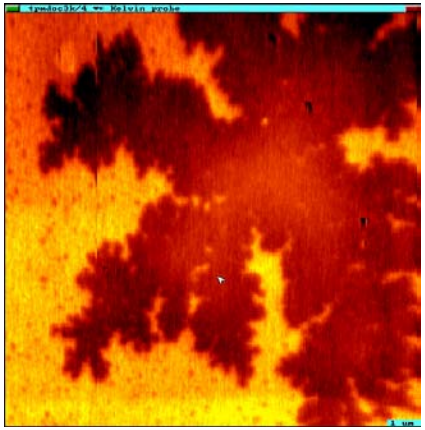


Model:



Result 3: effect of humidity on C18 alkylsilanes on Si wafers

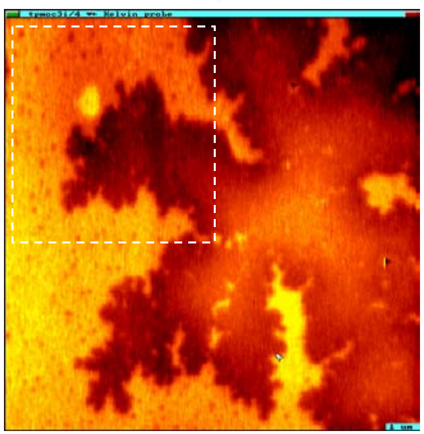
11%

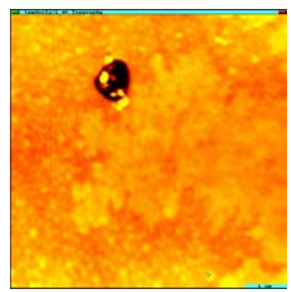


Water does penetrate near edges of islands, as shown by changes in contact potential at the island periphery

10 × 10 μm

80%





Contact tapping

New theoretical and computational advances

FS-MRL,SNL/NM, ORNL, PNNL, Vanderbilt

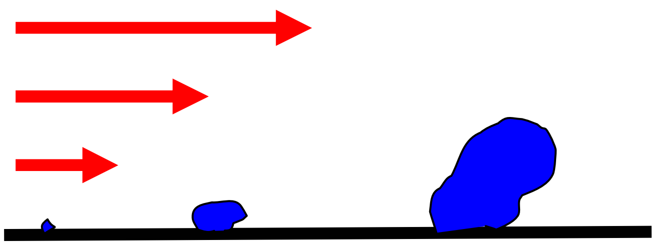
Manipulating the Boundary Condition of Fluid Flow in Micro- and Nanochannels

Granick et al. Nature Materials (2003) 2, 221. Presently complemented by work at Sandia (Grest, Stevens, Dugger).

Novelty: **Fluids flow between single crystals that are free of steps, allowing the surface chemical influences on flow to be disentangled from those of surface roughness.**

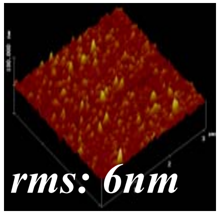
The Problem:
Commonly fluids come to rest at a moving surface.

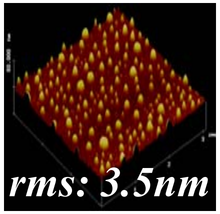
How moving fluid meets a solid

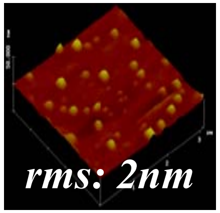


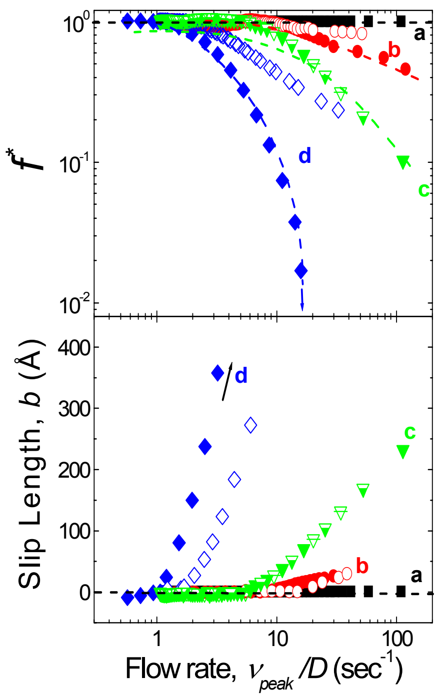
Energy Relevance: **Rational designs for saving energy during fluid flow in microchannels and MEMS devices. Has also suggested new hypotheses of how to scale-up to flow in macroscopic-sized pipes.**

Key Result: **The classical "stick" condition of viscous flow in textbooks can fail – severely. Moreover, the actual situation can be manipulated by rational minimization of surface roughness.**



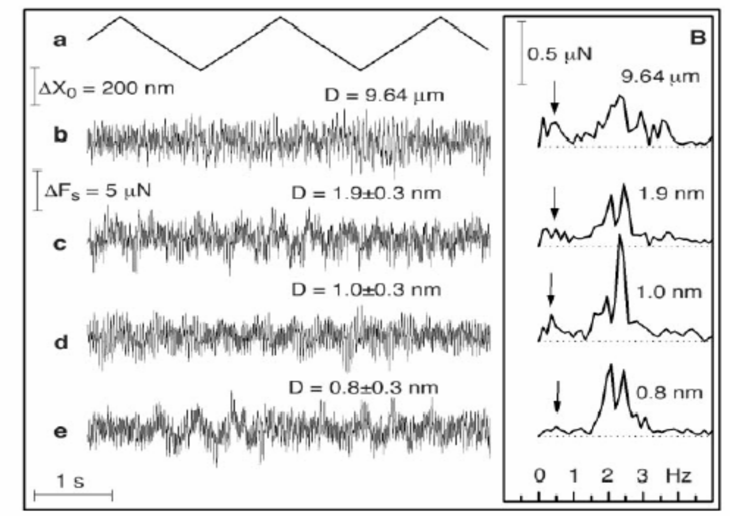


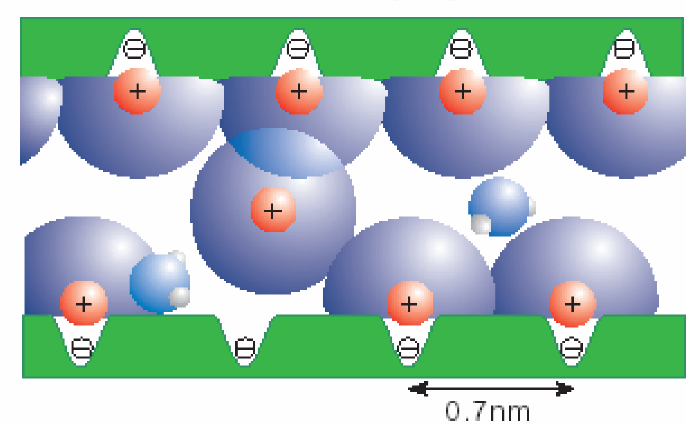




- **Properties of hydration water nanoconfined between mineral surfaces (e.g. muscovite mica):**
  - Nanotribology — structure and friction dynamics under extreme confinement
  - Geochemistry and Earth Science — clay swelling
  - Biological process — charge migration in living system

❑ **Surface Force Balance(SFB) experiments:**



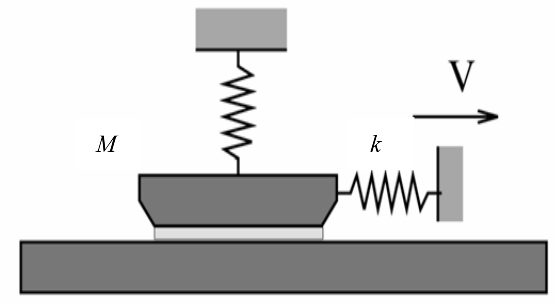


Raviv and Klein, *Science*, 297, 1540 (2002)

❑Mechanical model

Simulation parameters:

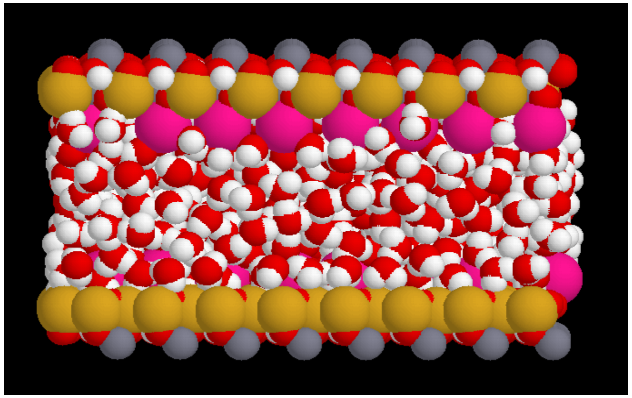
M=2000[O]=32000amu=5.344×10^{-23}kg; k=300N/m;
Sliding velocity v=10~400m/s; Applied pressure p = 1.0 atm; T=298K, time step Δt= 2fs.

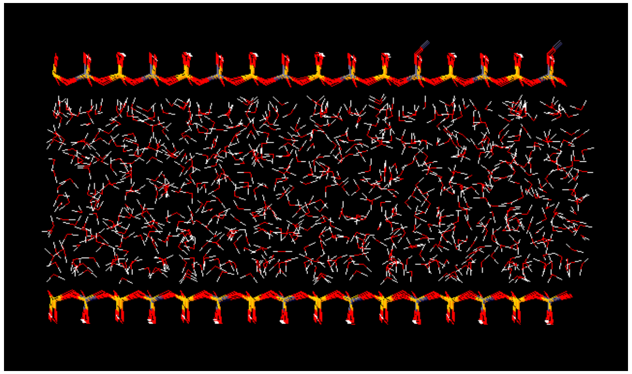


Results

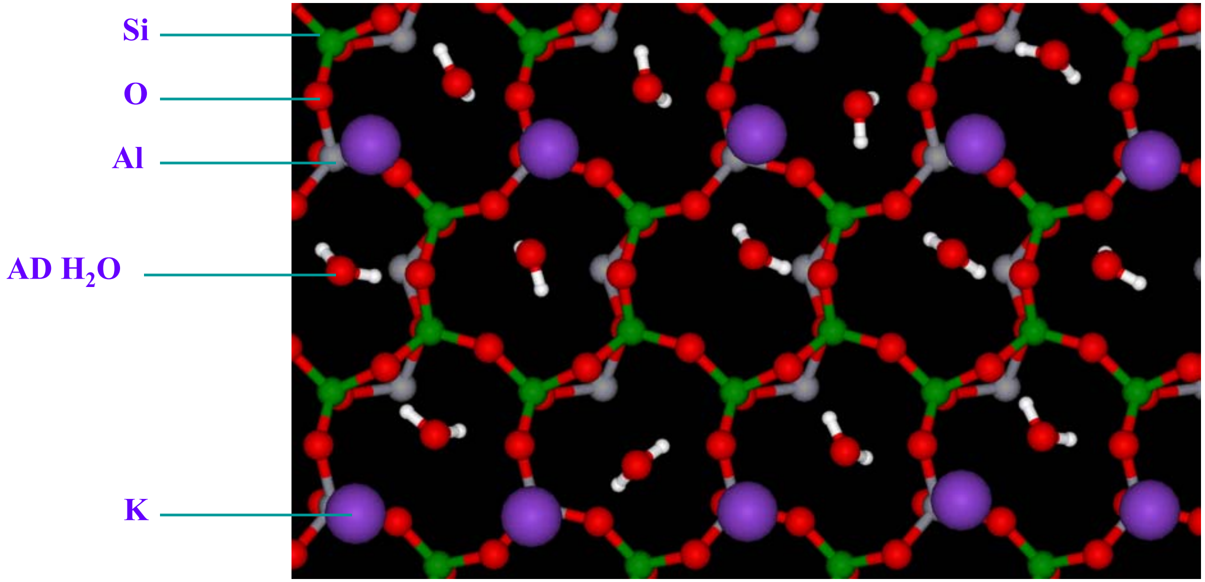
Structure of the hydration water

A. K^+ mica:

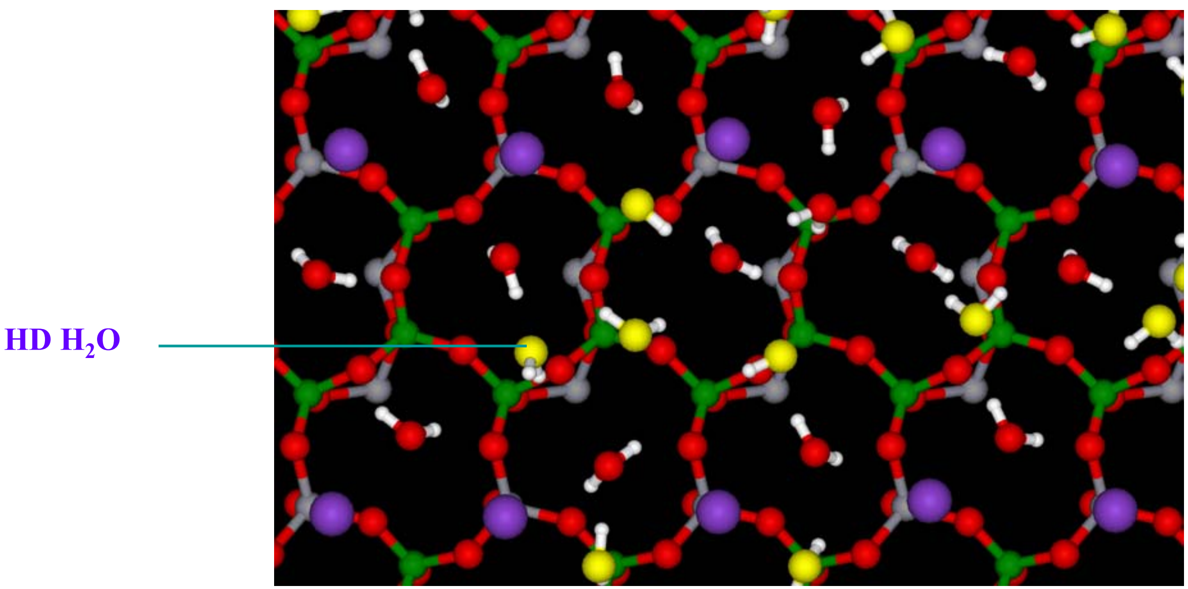




768 water, 64 K^+ (D=1.75nm) (n=6)

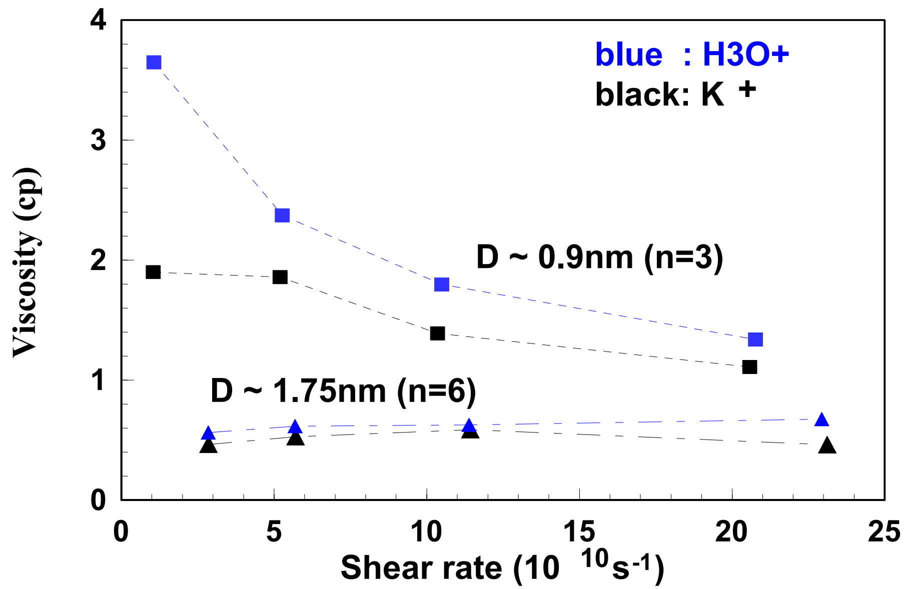


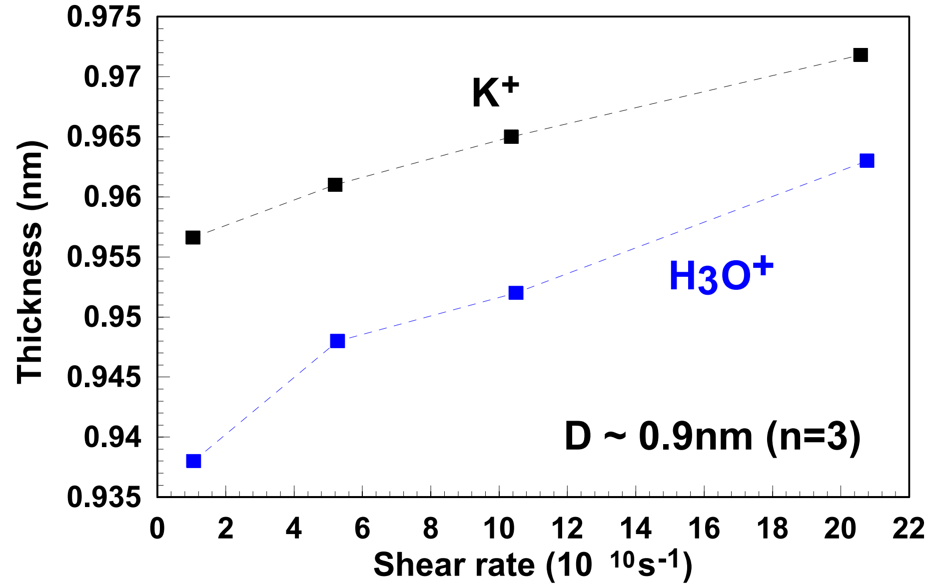
Adsorbed (AD) water layer structure



Adsorbed + the first hydration(HD) water layer structure

Shear viscosity





Shear thinning and dilatancy for n=3 water films

Friction dynamics

No stick-slips even for n=3 water layers (D<1.0nm)

For n=6 water layers, shear viscosity already approach the bulk value

For water layers thinner than 1.0nm, the shear viscosity is approximately 2~4 times of the bulk value, consistent with SFB experimental results

Thinner water films (D<1nm) between H3O+ mica surfaces result in a comparably higher viscosity

Adsorption structure of water near mica surface

O density oscillations near K+ mica surface are similar to the x-ray experimental curve. However, when K+ ions are exchanged by H3O+, the O adsorption peak is much higher than x-ray experimental value

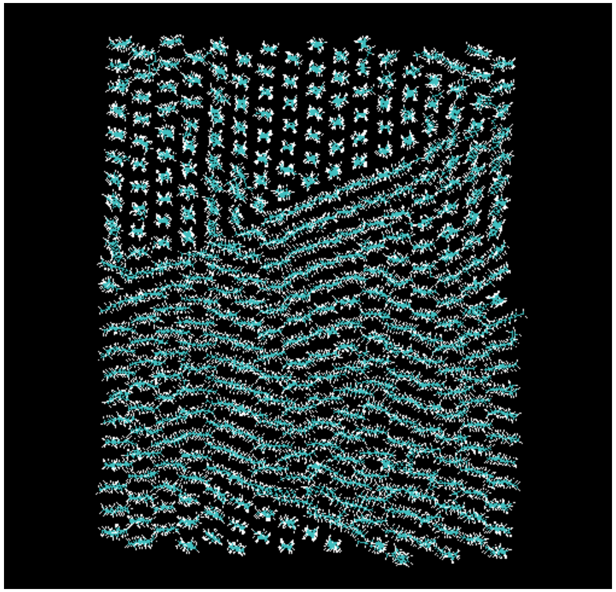
Adsorbed water molecules are basically attached to the ditrigonal cavities with their dipoles pointing towards the mica surface

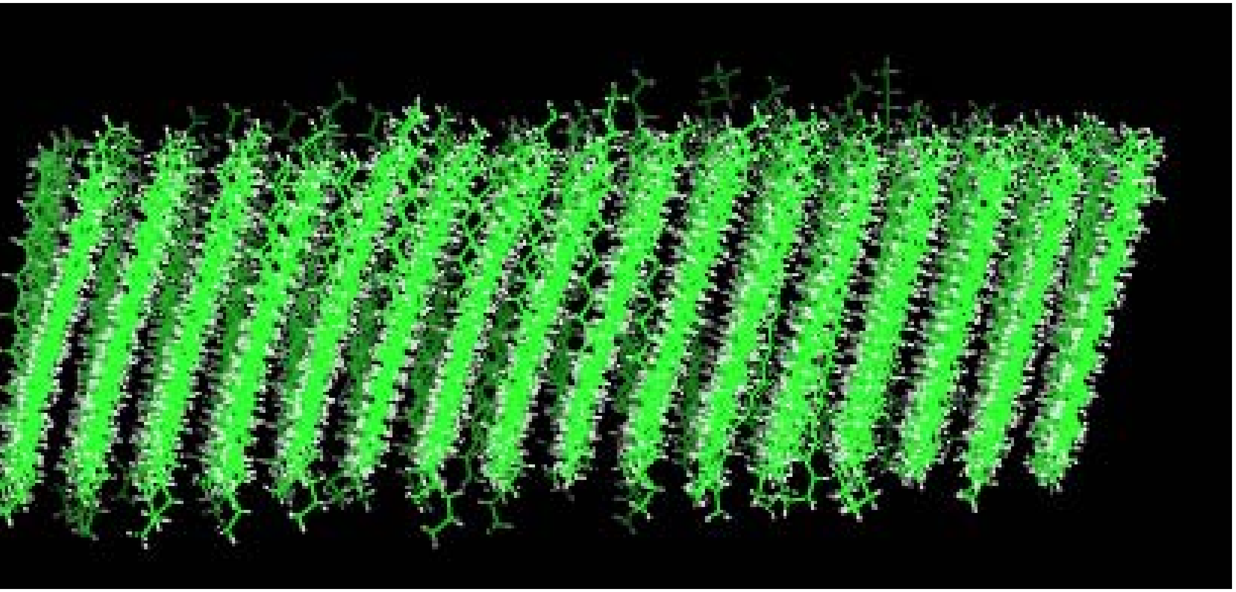
Molecular Dynamics Simulations of OTS Monolayer Films Based on AMBER Force Field: Comparison with X-Ray Scattering Measurements

368 OTS molecules (20608 atoms), area/molecule fixed at 19.6 Å^2

- Silica substrate is not included, very stiff compared to OTS
- Roughness at silica-OTS interface simulated by fixing the terminal OTS hydrogen atom at the surface about a mean position with Gaussian distribution
- After initial minimization, simulation was run for 2 ns at 300K

TOP view, showing domain formation, σ = 2 Å roughness.





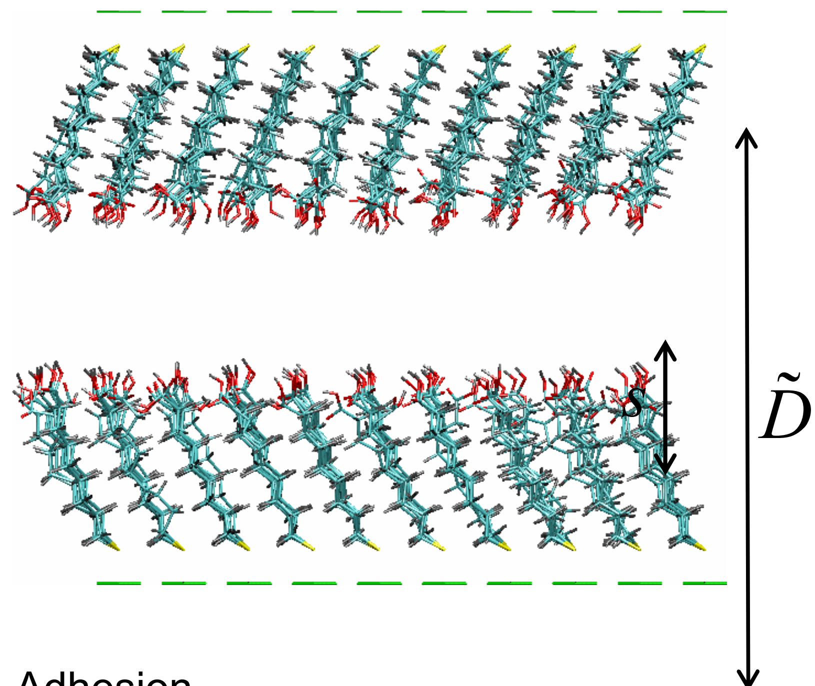
SIDE view, showing that molecules“lean”.

F. Trouw, et al.(LANL)

Los Alamos NATIONAL LABORATORY

Adhesion and Friction Simulations

- Two apposed SAMs
  - coated tip
- Adhesion
  - bring together at constant velocity (~ m/s)
  - equilibrium runs at specific separations
  - relative displacement, *D*
    - $D = s$ at 10Å
- Friction
  - shear at constant velocity under a load, $P_{\perp}$



Adhesion

See stronger attraction due to hydrogen bonds

Odd chain length stronger than even

Difference decreases with chain length

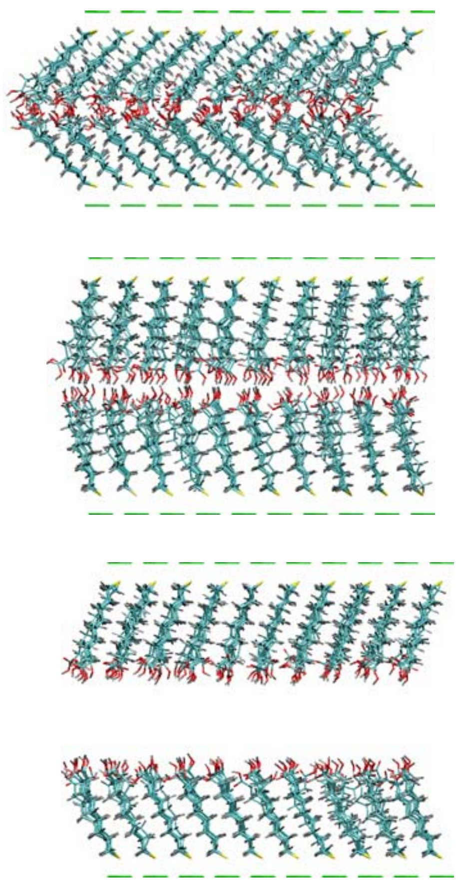
Stevens, Chandross, and Grest

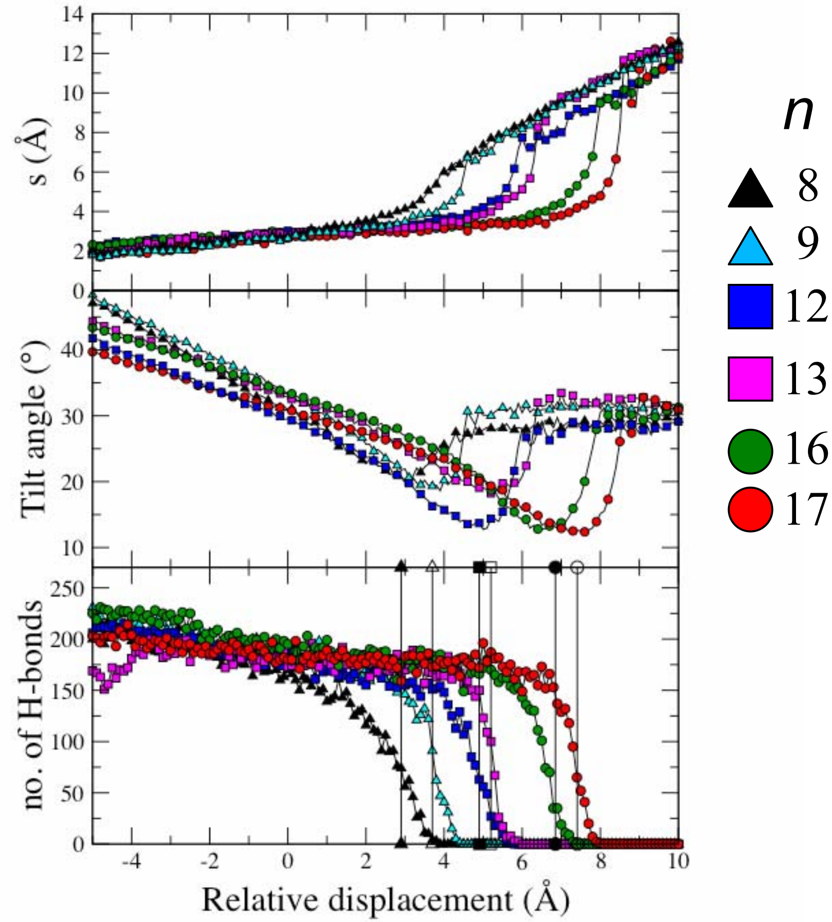
Structural Changes

D = -4Å

D = 3Å

D = 10Å





Stevens, Chandross, Grest

Comparison of Friction Coefficients

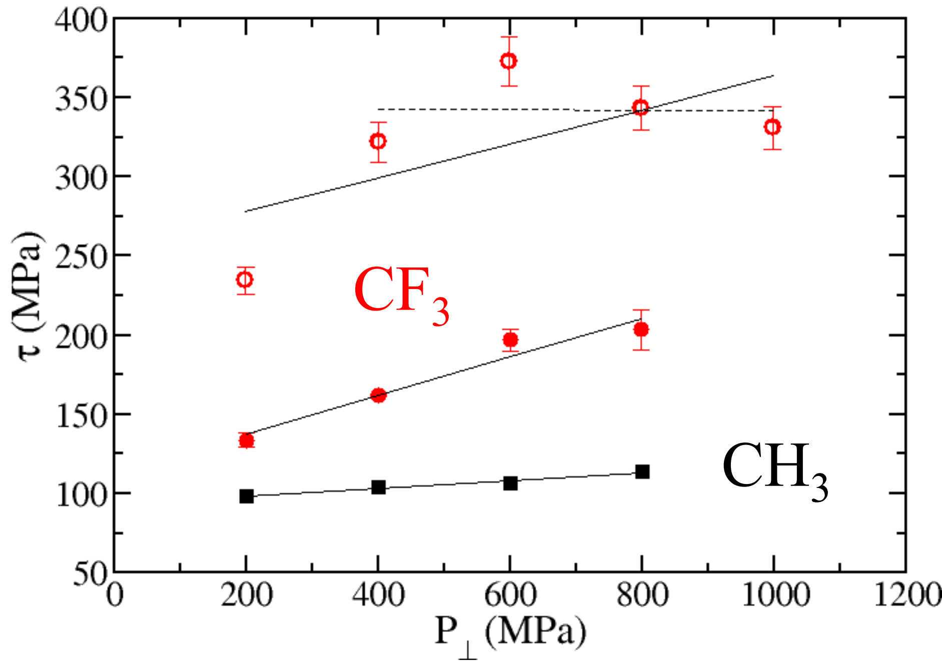
- Calculate μ from slope of shear stress vs. load curve
- Find $\mu(CF_3) > \mu(CH_3)$

0.12±0.02

0.03±0.01

0.10±0.07 ?

- Why two sets of CF_3 data?



Friction

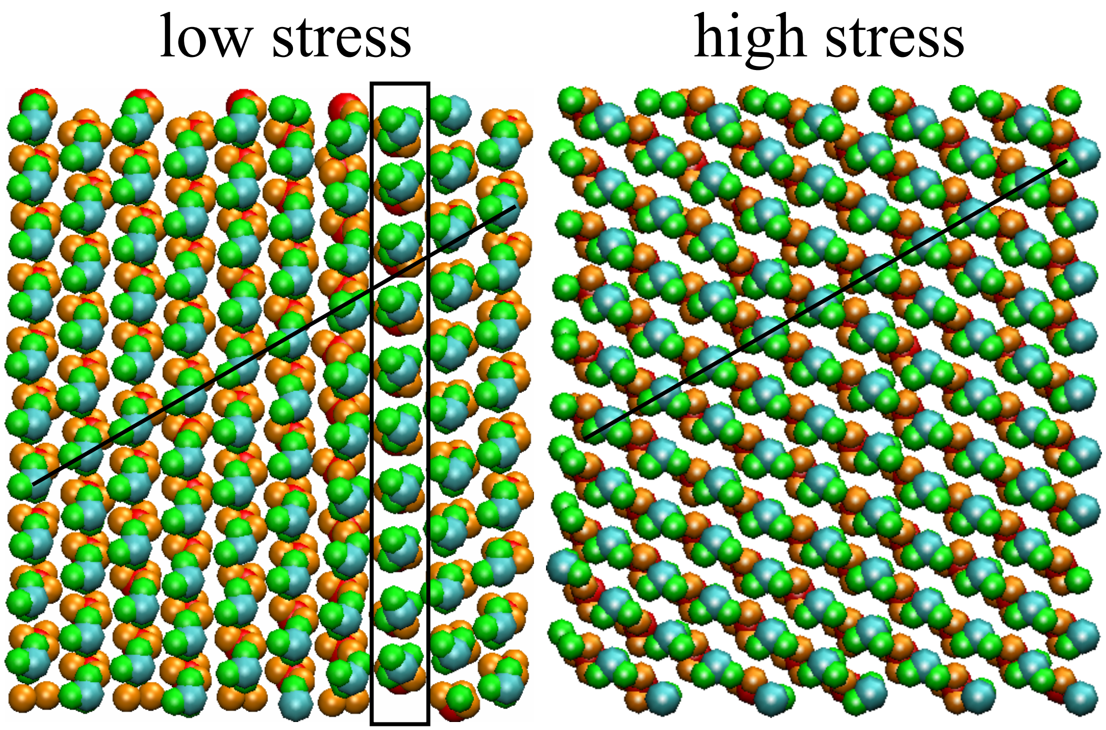
$m(CF_3) > m(CH_3)$

WHY? packing certainly relevant
need simple models of friction
(load dependence) line defect
occurs in CF_3 SAMs

Stevens, Chandross, Grest

Why High & Low Shear Stress for CF_3?

- Low stress case has a line defect
  - – a line of CF_3 slides *over* the line below
- High stress case is well ordered



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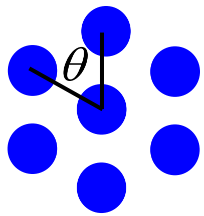
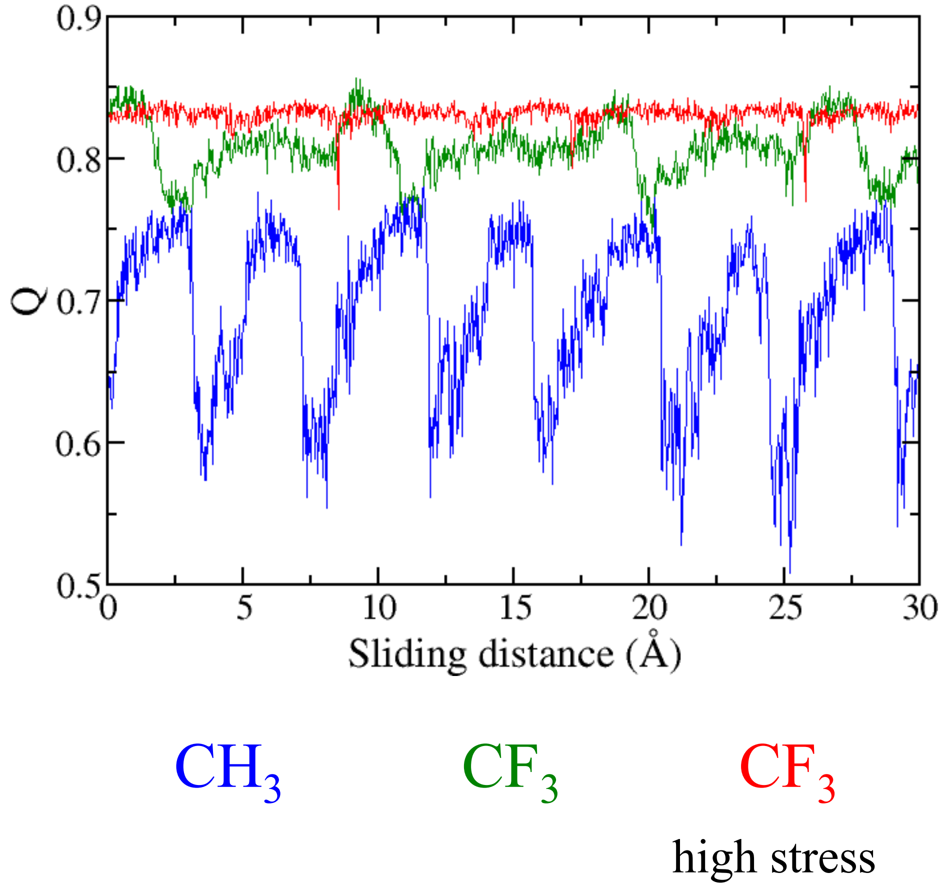
Order in Monolayer under Shear

- Calculate the hexatic order parameter,

$$Q = \frac{1}{N_6}\sum \exp(6i\theta)$$

- High stress CF_3 has largest Q
  - predominantly constant
- Both CF_3 have larger Q than CH_3





Stevens, Chandross, Grest

Collaborations:

Mike Dugger + Miquel Salmeron = SPFM studies of OTS coated MEMS

Steve Granick + Miquel Salmeron = Development of spectroscopic tools for studies of buried interfaces

Ali Erdemir + Sunil Sinha = Development of surface coatings for ultralow friction

Yehuda Braiman + Marten de Boer + Robert Carpick = Stick-slip in MEMS, lubrication control

Additional common points of interest evolving:

ORNL – SNL (Effects of disorder on sliding, MD and modeling)

ANL – ORNL (Ultralow friction)

More ongoing group activities

Peter Cummings: molecular dynamics simulations of water nano-confined between mica sheets

Michael Kent, Mike Dugger (SNL): neutron reflection experiments (@NIST) to detect water at the interface between SAM lubricants and silicon oxide. Kinetics of hydrolysis of Si-O-Si and rate of degradation of the SAM lubricants in high temperature high, humidity environments

Park, Chandross, Stevens, Grest. (SNL): effect of water on chain conformations and mechanical properties of SAM

…/…

Workshop at ORNL
March 11-13, 2004

This workshop will delve into the scientific richness of the field of tribology and lubrication, espeically the nanoscale aspects of these fields. Emphasis will include the range of multiscale phenomena, complexity in physical and chemical behaviour, and economic impact. A white paper will be generated from issues explored at this meeting.

Invited speakers include:

Adnan Akay (CMU)
Maarten De Boer (Sandia)
Peter Blau (ORNL)
Yehuda Braiman (ORNL)
Robert Carpick (UW Madison)
Peter Cummings (Vanderbilt)
Mike Dugger (Sandia)
Ali Erdemir (ANL)
Steve Granick (UIUC)
Garry Grest (Sandia)
Jacob Israelachvili (UCSB)
Shaoyi Jiang (U Washington)
Joseph Klafter (Tel Aviv)
Jacob Klein (Oxford/Weizmann)
Jackie Krim (NCSU)
Uzi Landman (Georgia Tech)
Yongsheng Leng (Vanderbilt)
Scott Perry (U Houston)
Seth Putterman (UCLA)
Miguel Salmeron (LBL)
Sunil Sinha (UCSD)
Mark Stevens (Sandia)
Thomas Thundat (ORNL)

Organizers:
Y. Braiman (ORNL), P. Cummings (Vanderbilt), S. Granick (UIUC)

More information can be found at:
http://www.csm.ornl.gov/meetings/FiTAS

Draft

WHITE PAPER

Frontiers in Tribology at the Atomic and Nano Scales

Prepared by

Y. Braiman, ORNL

P. Cummings, Vanderbilt University and ORNL/CNMS/NTI

S. Granick, FS-MRL

May 18, 2004

Friction between surfaces in contact constitutes a long standing very important science problem. It involves interplay between energy, chemistry, material science, physics, mathematics, and engineering fields and unites scientific and technological needs. On the scientific side are fundamental questions of how energy is dissipated in non-equilibrium processes, for example of how the course of this energy dissipation can be intentionally controlled using modern theories and advanced control circuitry. Other fundamental scientific questions concern the structure of surfaces, especially of surfaces buried beneath macroscopic-sized phases – the scientific challenge here is to do great surface science, but outside the conventional conditions of UHV.

Timeliness of New Investment

- New and exciting theoretical insights, occasioned as the attention of world-class theorists has become directed to this problem that in the past tended to be dismissed as "dirty" and "too applied" by the best theorists.
- Unprecedented capabilities for physico-chemical characterization, among them the advent of laser-based chemical characterization technologies and the application of user-based facilities such as high-generation synchrotron sources, which did not exist previously. The main point of these characterization tools is the unprecedented capacity to measure directly, *in situ*, what is actually happening in these ubiquitous sliding contacts between moving surfaces.
- Unprecedented new computational facilities and advances in algorithms and methodology afford obvious other capabilities that can be directed to this field;
- Unprecedented new experimental horizons based on recent DOE investments in new instrumentation (e.g., the Spallation Neutron Source and the APS). The key new point is the unprecedented capability to design, control, and analyze, with full control over the relevant physical and chemical features, the physical makeup of the moving parts.
- The unprecented advent of novel experimental devices and novel tools to measure and control frictional properties of the sliding surfaces

Outstanding Scientific Challenges

- How to advance conceptual advances and breakthroughs (e.g., broadly applicable equations for friction and friction-wear relationships), using newly developed experimental methods that enable direct observation of what is happening at contact.
- Experimental and theoretical elucidation of the linear character of friction (at and near equilibrium), and its relation to modern statistical-mechanical theories of solids and liquids at equilibrium, in the fields of modern physics, chemistry, and mechanics.
- Elucidation of the nonlinear character of friction (far from equilibrium). Extend definitively this challenging problem to modern experimental frontiers of definitive analysis; to modern theories of complexity; and to modern computational resources.
- Explanations of how lubricant fluids avoid the development of prohibitively high forces when rapidly driven far from equilibrium? It seems clear that there is no single mechanism and that solutions to this problem will bring the field into closer contact with emerging questions of polymer processing and, more generally, the boundary conditions for fluid flow over a surface.
- If we now move out of steady-state conditions, how does a soft fluid respond to a high-amplitude, short-lived change in pressure, deformation rate, or compression?

Outstanding Scientific Challenges

- No one yet really knows whether a general theory of surfaces in sliding contact is possible. The flow of confined fluids is very much like granular materials such as sand, powder, and colloidal particles. Too often the models are system-specific -- but common responses strongly suggest more universality, which could reflect the fact that high density, short-range packing, and dynamical rearrangements of structure by instability are so interrelated.
- Can we predict, from theory rather than empiricism, what makes lubricant molecules of one chemical structure more effective in lowering friction forces than another?
- Recurring themes in discussions of outstanding problems are: Friction and lubrication at extreme conditions (such as high-temperature or nonequilibrium or nanoconfinement), phenomena still to be understood (stick-slip boundary conditions at the macroscale, tribo-charging, triboluminescence, and the general problem of quantum effects in tribology), and the performance of whole tribosystems (based on their constituent parts).
- How to design tribological surfaces with given frictional properties (i.e., principles for surface engineering)? How to deliberately and controllably change frictional properties while sliding, leading to intentional control of friction?

Needs for Investment

DEVELOPMENT OF NOVEL EXPERIMENTAL TECHNIQUES AND DEVICES TO MEASURE AND CONTROL FRICTIONAL PROPERTIES OF THE SLIDING SURFACES.

Need for in-situ evaluation of chemical and physical processes that occur during processes far from equilibrium. The traditional approach of force (friction) measurement needs to be augmented using newly available opportunities for diagnosis at the atomic and molecular levels, for example using laser-based diagnostic methods. Among the most promising such resources are application of technologies that come from other fields of study that enable sophisticated optical and spectroscopic characterization. Other important advances will involve DOE-sponsored facilities, such as the APS and the neutron spallation source. In the first category, there is great untapped potential for characterization using methods of fluorescence spectroscopy, of linear vibrational spectroscopy (e.g. Raman) and of nonlinear vibrational spectroscopy (e.g. sum-frequency generation), that are already developed to a high level of sophistication in other fields such as physical chemistry and biophysics, but have hardly been applied to the more challenging tribological problems of surfaces in moving contact.

Needs for Investment

MODELING AND SIMULATION.

Unprecedented increase in computer capabilities opens new trends in modeling and understanding of tribological properties of materials. The ability to model and visualize large-scale systems under confinement provides a powerful prediction tool that is capable of guiding and analyzing experimental research in the environment of the limited access. Atomistic molecular dynamics (MD) simulations are currently limited to time-scales no greater than tens of nanoseconds and lengths scales of tens of nanometers, which are too short for analyzing variety of tribological systems. Development of new algorithms and new computational tools (such as parallelization and vectorization) will result in significant increase in time scales for MD simulations on friction. Additionally, new ultra-scale computing resources make it possible, for the first time, to consider the impact of reactions at lubricant–surface interface and surface reconstruction effects, using *ab initio* MD.

Needs for Investment

ULTRA THIN FILM LUBRICATION.

Of specific opportune importance is the problem of thin-film lubrication, which traditionally was hardly studied but has become important for a number of reasons. First, lubricant films in conventional machine components are becoming thinner in recent years. The quest for energy efficient systems drives the use of lower viscosity lubricants. At the same time there is increasing demand for reducing maintenance, and therefore for improved lubricant durability. New synthetic lubricants are needed for some of the demanding applications and new additives will be required to enable low friction, low wear operation in mixed lubrication conditions.

STICK AND SLIP AS CONTROLLABLE BOUNDARY CONDITIONS.

Recently, the revolutionary idea became recognized that the boundary condition when a flowing fluid meets a solid boundary can be put under an experimentalist's control. It now appears to be feasible to design solid surfaces, mediated by intervening fluids that flow past one another such that the friction occasioned by this process is orders of magnitude less than supposed by standard textbook accounts. The ideas and proofs-of-concept exist … but full understanding and rational implementation are at an early stage.

Needs for Investment

DESIGN OF SURFACES WITH GIVEN FRICTIONAL PROPERTIES.

Surface design has been of growing importance in the past decade and will continue to be critical in the future. New coating technologies have been developed in recent years which have enabled the production of surfaces which are harder, more durable, and more functional than the substrates beneath them. As these developments spread throughout the technical community, the design of surfaces will become as important as the choice of the substrate material. For example, clear opportunities exist with the potential for deliberate control and manipulation of friction, not necessarily by the traditional chemical means (by supplementing base lubricants with friction modifiers additives), but instead by implementing a bridge between known theoretical/numerical algorithms and experimental implementation. The key needs are accessibility and speed of control.

Relevance to the DOE Mission

As concerns technological impact, we note that friction and wear are estimated to cost the US economy 6% of the gross national product. In a $12 trillion GNP, this translates to over $700 billion per year. For example, 5% of the energy generated in automobile engines is lost to frictional resistance. Also notable are many tribology issues in the human body. To summarize the energy-related functions that would be served by advances in nanoscale friction:

- Less energy lost unnecessarily in machines. The total possible savings is measured not in fractions of a percent, but at the important level of several percent of the GNP.
- Less energy lost unnecessarily in health cost. These are not under the purview of the NIH because the moving parts in the human body undergo much friction even in the absence of disease. The possible gain in terms of standard of life is inestimably large.
- Enabling technology for MEMS-related devices. The development of durable and /or low friction surfaces and ultra thin lubrication films has become an important factor in the miniaturizing of moving components in many topical technological devices. Progress in these technologies is widely acknowledged to be rate-limited by obstacles related to moving contacts.